THREE-DIMENSIONAL SUPERCELL SIMULATION OF QUANTUM TRANSPORT

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Abstract

Three-dimensional quantum transport is examined with a supercell one-band tight-binding model. Unlike conventional 1D quantum transport calculations which account only for variation along the transport direction, our model accounts for lateral variation as well. This flexibility allows us to examine such topics as alloy disorder, interface roughness and other fluctuation phenomena in a diversity of systems such as double barrier resonant tunneling (DBRT) structures, quantum wires, quantum waveguides and other semiconductor heterostructure systems that hold technological promise. The model can also be extended to include more realistic multiband band structures.

In this paper we employ the model to investigate alloy disorder in DBRT structures. Shifts and broadenings of the transmission resonances of these structures are clearly seen when compared with Virtual Crystal Approximation (VCA) calculations, which do not address alloy disorder. These differences are reflected in the J-V characteristics. Increased peak current and a reduced peak-to-valley ratio are evident in the 3D supercell simulations. In addition, the peak current is shifted to lower bias.

THEORETICAL MODEL

We use a supercell scheme in conjunction with the tight-binding picture. In our tight-binding formalism, a structure consists of a collection of sites on a cubic lattice. In the one-band model an onsite energy is associated with each site, and a transfer matrix element is associated with each nearest neighbor pair of sites. In pure materials these are related to the conduction band edge and effective mass of the materials, respectively.

In the supercell scheme, a structure is represented as a collection of layers normal to the transport direction. Each layer consists of a periodic array of identical supercells one lattice unit cell thick and several lattice unit cells on an edge. The types of lattice sites within a supercell depend on the structure under consideration. To model a disordered binary alloy layer, for example, the supercell for that layer would contain a disordered distribution of two types of sites.

To calculate transport through the structure, we first set up the boundary conditions. This is accomplished by calculating the electron eigenstates in the left and right electrodes in terms of the

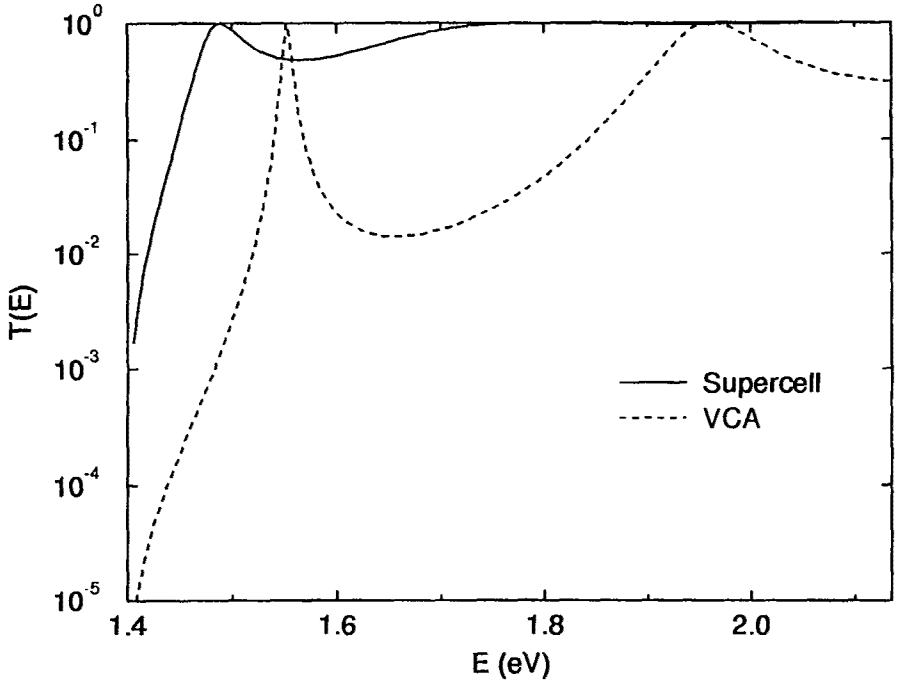

Figure 1: Transmission coefficient for a DBRT structure with 5 ml alloy disordered barriers and a 15 ml pure well. Comparison of supercell and VCA calculations.

tight-binding orbitals. We then feed this information, along with the onsite energies and transfer matrix elements into a system of linear equations which we solve for the electronic wavefunction throughout the structure[1]. This method is just as efficient as the transfer matrix method and does not suffer from the numerical instability which plagues the latter.

Having solved for the electronic wavefunction in the structure, we calculate the transmission coefficient based on the form of the wavefunction in the right electrode. To derive J-V characteristics, the transmission coefficient is integrated over the Fermi distribution and over all possible in-plane momenta[2].

SIMULATION RESULTS

We first apply the model to a DBRT structure with disordered binary alloy barriers. We take the barriers to be 5 monolayers thick, consisting of 30% well-type material and 70% barrier-type material. The well is pure material 15 monolayers thick. The electrodes also consist of pure well-type material. We assume a lattice constant of 2.825Å throughout, a barrier effective mass of $0.1248m_0$ and band edge of 2.48 eV, and a well effective mass of $0.0673m_0$ and band edge of 1.43 eV, parameters typical of AlGaAs. We have performed both a VCA calculation and a 3D supercell calculation of the transmission coefficient at zero in-plane momentum for this structure. For the supercell simulation, we used a square supercell 15 lattice unit cells on an edge. Figure 1 shows the results. The supercell simulation shows substantial broadenings and shifts of the transmission resonances when compared with the VCA calculation, which does not treat disorder.

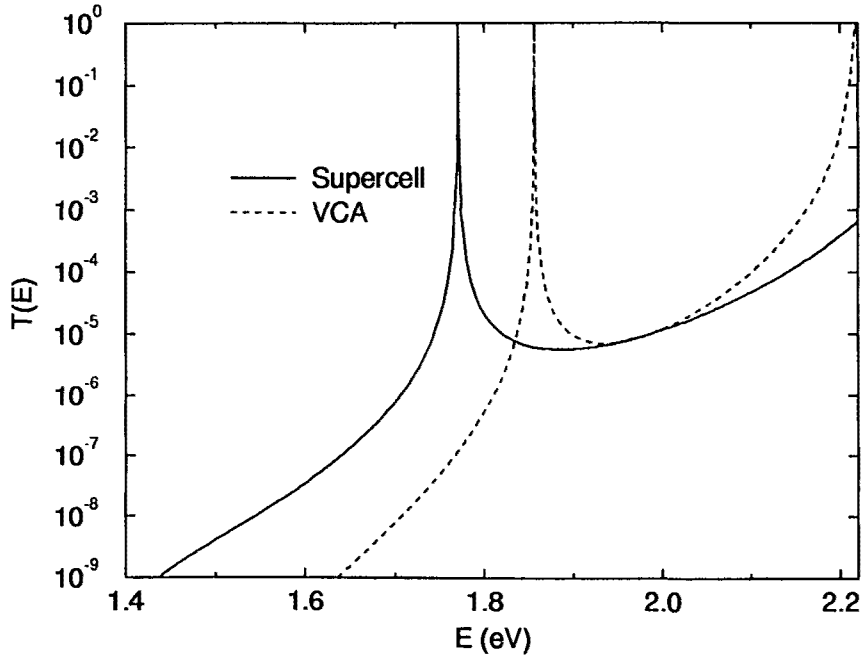

Figure 2: Transmission coefficient for a DBRT structure with 10 ml pure barriers and a 15 ml alloy disordered well. Comparison of supercell and VCA calculations.

The model is next applied to a DBRT structure with a disordered well. The results are shown in Figure 2. The same parameters as above apply, except that here the barriers are 10 monolayers of pure material, and the well is 70% well-type material and 30% barrier-type material. There again appears a substantial shift in the resonance. The shifts and broadenings in these cases are due to the complex self-energy[3] arising from the large disorder potential implied by the material parameters assumed in this one-band model.

The effects of disorder can also be seen in J-V characteristics. Figure 3 shows zero temperature J-V curves for a DBRT structure with 5 monolayer barriers and a 15 monolayer well. The well is pure and the barriers consist of the same type of alloy as above. The supercell simulation shows higher peak current and lower peak-to-valley ratio than that of the VCA calculation. The peak is also shifted to lower bias. The J-V curve shift results from the corresponding shift in the transmission coefficient curve, and the increased peak current and reduced peak-to-valley ratio reflect leakage through the disordered barriers.

CONCLUSION

We have demonstrated a model for performing 3D supercell quantum transport calculations. We have used the model to calculate transmission coefficients and J-V characteristics in alloy disordered DBRT structures. Substantial disorder-induced broadenings and shifts in the transmission coefficients are evident. These effects can also be seen in the J-V characteristics. We hope to investigate many more interesting nanostructure phenomena with this flexible, efficient model and

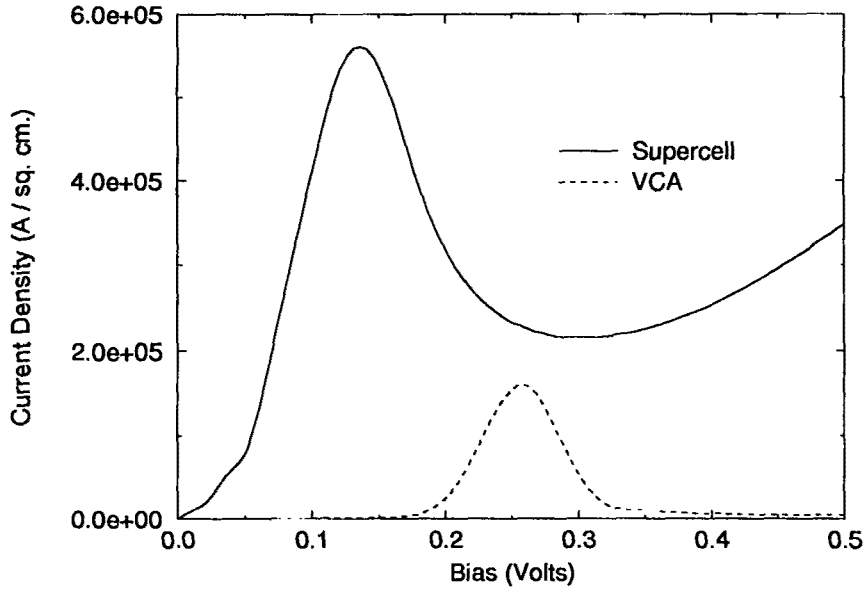

Figure 3: J-V characteristics at zero temperature for a DBRT structure with 10 ml alloy disordered barriers and a 15 ml pure well. The electrode fermi level is 0.05 eV above band edge.

to extend it to incorporate more realistic band structure in future publications.

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